Characterization of 3d topological insulators by 2d invariants

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Abstract

The prediction of non-trivial topological phases in Bloch insulators in three dimensions has recently been experimentally verified. Here, I provide a picture for obtaining the Z_2 invariants for a three dimensional topological insulator by deforming suitable 2d planes in momentum space and by using a formula for the 2d Z_2 invariant based on the Chern number. The physical interpretation of this formula is also clarified through the connection between this formulation of the Z_2 invariant and the quantization of spin Hall conductance in two dimensions.

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Insulators with weak inter-electronic interactions in crystalline materials are well described by band theory. The energy eigenstates can be grouped into Bloch bands and the presence of a gap at the Fermi energy prevents charge transport in the bulk since filled bands do not contribute to electronic transport. Since the discovery of the quantum Hall effect,[1] however, it has been known that materials which have a bulk gap in their single particle spectra may nevertheless have gapless edge modes, through which charge transport may take place. Various theoretical studies, an incomplete list of which includes Refs. 2–6, have helped to explain the quantization of the conductance, the connection between the bulk Hamiltonian and the Hall conductance and the robustness and role of the edge states in the quantum Hall effect.

Recently, a set of novel topological phases which are somewhat similar to the quantum Hall phases have been proposed to exist in ordinary insulators with unbroken time reversal symmetry(TRS). (From here on, unless stated otherwise, we shall restrict ourselves to a discussion of band insulators with unbroken time reversal symmetry.) In two dimensions, there are two distinct topological phases[7] characterized by a single Z_2 invariant, while in three dimensions, sixteen topological phases characterized by four topological Z_2 invariants[8,9,11] have been proposed to exist in non-interacting systems. These topological phases have been detected in HgTe quantum wells surrounded by CdTe in two dimensions[12,13] and in $Bi_{1-x}Sb_x$ alloys in three dimensions[14,15] among other compounds. Like in the quantum Hall effect, the topologically non-trivial phases of insulators with TRS have gapless edge modes which are robust to small perturbations. Topological phase transitions between these phases have been studied in Ref. 16.

While in two dimensions, the analogy with the integer quantum Hall effect leads to a simple picture for the topological phases and the Z_2 invariant, in three dimensions, the picture is far more complicated. This is in part, due to the fact, that unlike the integer quantum Hall effect, in 3d materials with unbroken TRS, while three of the Z_2 invariants are analogous to the 2d Z_2 invariants, there is a fourth Z_2 invariant which is intrinsically three dimensional.

Insulators with a non-trivial value of this fourth invariant have a description in terms

of an effective field theory containing a θ term which successfully describes the physics of the boundary[17]. In this work, I provide a different argument for counting the number of different topological invariants and thus the number of different topological phases in three dimensional insulators. Since the picture relies on invariants for two dimensional topological insulators, I will briefly review this case as well. A physical interpretation of the invariant as formulated in terms of Chern numbers in two dimensions is also provided.

I. TWO DIMENSIONS

The original approach to the topological invariant in two dimensions was based on counting the zeroes of a function calculated from the Pfaffian of a certain matrix[7]. A different approach developed by the author was based on the obstruction of the vector bundle of wave-functions on the torus to being a trivial bundle[18]. This yielded a formula involving the Chern number of half the occupied bands. Subsequent work using the obstructions approach and physical ideas related to charge polarization led to a formula involving an integral of the Berry curvature of all the bands, but restricted to half the Brillouin zone (also called the effective Brillouin zone(EBZ))[19]. In other related work, the topological phases in two dimensions were studied by deforming maps from the EBZ to the space of Bloch Hamiltonians with unbroken TRS, $\mathcal{C}$, to maps from a sphere or a torus to $\mathcal{C}$ (Ref. 8). The formula involving the integral over the EBZ in Ref. 19 has been adapted to numerical evaluations[20], while the formula in terms of the Chern number has the advantage of having a direct link to the edge state physics and the integer quantum Hall effect. A brief review of the latter formulation is provided below.

The Hamiltonian of a Bloch insulator has single particle eigenstates, which are either occupied or unoccupied depending on their energy relative to the Fermi energy. The spectral projection operator is defined as the operator that projects single particle states onto the space of occupied states. It can thus be written as sum, $P = \sum_i |u_i\rangle\langle u_i|$, where the $|u_i\rangle$ are the occupied eigenkets. Thus the projection operator can be written as: $P = \sum_{k_x,k_y} P(k_x, k_y)$ where the sum is over reciprocal lattice vectors lying in the Brillouin zone.

As was argued in Ref. 18, in materials with time reversal symmetry the spectral projector, P can be written in the form:

$$P(k_x, k_y) = P_1(k_x, k_y) + P_2(k_x, k_y) \tag{1.1}$$

where the operators, P_1, P_2 are well-defined, continuous functions of the momentum variables and are related through time reversal symmetry:

$$P_1(k_x, k_y) = \Theta P_2(-k_x, -k_y)\Theta^{-1}$$

Here, Θ is the time reversal operator which acts on the spin degrees of freedom and is anti-linear. The choice of P_1 and P_2 is not unique. We further assume that P_1, P_2 can be chosen to be globally smooth. (See Refs. 10,18 .)

For every value of $\mathbf{k}$, $P(k)$ projects onto a complex vector space. We thus obtain a vector bundle over momentum space. The first Chern number of this bundle, which we denote by $\mu(P)$ can be written in the form[21],

$$\mu(P) = \frac{1}{2\pi i}\int dk_x dk_y Tr\left(P\left(\frac{\partial P}{\partial k_x}\frac{\partial P}{\partial k_y} - \frac{\partial P}{\partial k_y}\frac{\partial P}{\partial k_x}\right)\right).$$

The first Chern number vanishes for P in topological insulators due to time reversal symmetry, i.e., $\mu(P) = 0$. However, it was shown that $\nu(P) = |\mu(P_1)| \bmod 2$ is a topological invariant[18] and is independent of the choice of P_1.

Consider the subset of gapped Bloch Hamiltonians which conserve the z component of the spin, i.e., Hamiltonians in which there are no terms which turn up spins into down spins. The energy eigenstates can be decomposed into spin up and spin down bands. Hamiltonians in this class with a bulk gap will always have a quantized spin Hall conductance (which could be zero).

The Z_2 topological classification tells us that Hamiltonians of the even and the odd quantized spin Hall effects are distinct even when we allow spin mixing terms in the Hamiltonian. In terms of the spin Chern number C_s which can be defined for such models[22], the Z_2 invariant is $|C_s/2|$mod2.

In other words, if we allow terms which cause spin mixing, the Hamiltonians with an even spin Hall effect can all be transformed into one another through adiabatic changes in parameter space and those with an odd spin Hall effect can similarly be adiabatically transformed into one another. However, no member of the odd spin Hall conductance class can be transformed into any member of the even spin Hall conductance in a continuous way such that TRS is protected and the system is gapped at all points of the transformation. Further any general Bloch Hamiltonian (with the same Hilbert space and which has the same number of occupied bands) which preserves time reversal symmetry may be adiabatically transformed

to Hamiltonians of precisely one of the two sets of Hamiltonians without breaking TRS at any intermediate point. The trivial and non-trivial topological classes may be thought of as equivalence classes of Hamiltonians which contain respectively members which display an even and an odd quantized spin Hall conductance.

II. THREE DIMENSIONAL INSULATORS

The Brillouin zone for a 3D insulator has the topology of a three dimensional torus. We represent it by a cube $\{-\pi \leq k_x, k_y, k_z \leq \pi\}$. Under the operation of the TRS operator, a Bloch wave-function at the point $\mathbf{k}$ gets mapped to the point $-\mathbf{k}$. The plane in momentum space, $k_z = 0$ gets mapped onto itself under inversion and has the topology of a 2d torus. The spectral projector, P for the 3d insulator restricted to this plane, therefore has an associated Z_2 invariant.

There are a number of such surfaces with which one may associate a Z_2 invariant. A few of these are the planes $k_x = 0, k_x = \pi, k_y = 0, k_y = \pi, k_z = 0$ and $k_z = \pi$. The associated Z_2 invariants are denoted by $\nu_1, \tilde{\nu}_1, \nu_2, \tilde{\nu}_2, \nu_3$ and $\tilde{\nu}_3$ respectively. It was argued previously that the Z_2 invariants of these planes are not all independent[8,9,11]. The arguments were based on the counting of monopole charges[9], on contractions of the 3d EBZ to the 3d torus[8], or on the number of independent choices of time reversal polarizations[11]. Here, we provide a simple alternate argument for the number of independent Z_2 invariants in three dimensions. This argument also shows how the Z_2 invariants of planes such as $k_x + k_y = 0$ may be calculated from the other Z_2 invariants.

Consider the composite surface, S consisting of the shaded region in Fig. 1(a). This surface, which is a union of the two planes, $k_y = 0$ and $k_z = \pi$ can be mapped onto a two dimensional torus and is mapped onto itself under inversion. Thus, a Z_2 invariant may be associated with this surface. The projection operator for this surface can be written in terms of the two projection operators as:

$$P = P' \oplus P''$$

where P' is the projection operator restricted to the plane, $k_z = \pi$ and and P'' is restricted to the plane $k_y = 0$. Here, if $P' = \sum_{\alpha \in S'} |\alpha\rangle\langle\alpha|, P'' = \sum_{\alpha \in S''} |\alpha\rangle\langle\alpha|$, by $P \oplus P'$, we mean $\sum_{\alpha \in S' \cup S''} |\alpha\rangle\langle\alpha|$.

P, P' and P'' can be decomposed as in Eq. (1.1) and corresponding Z_2 invariants,

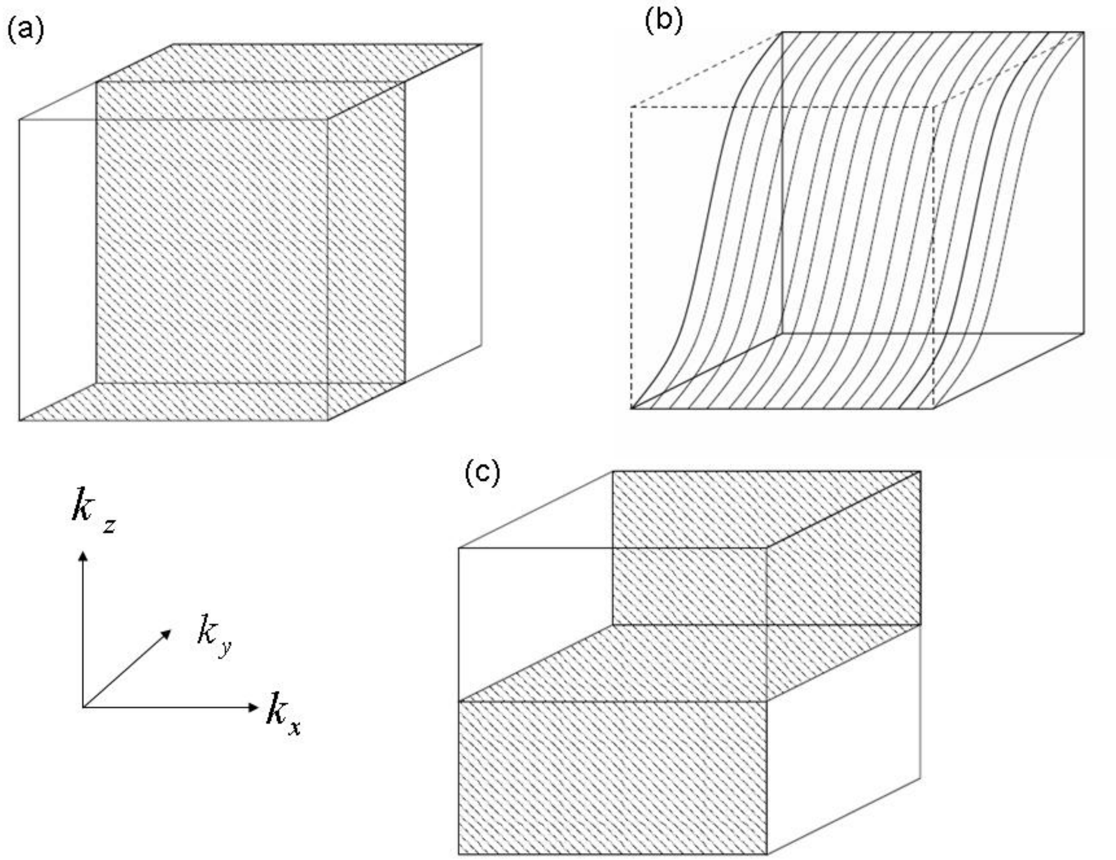

FIG. 1: The shaded region, S in (a) is the union of the planes $k_y = 0$ and $k_z = \pi$. This region can be continuously deformed into the shaded regions in (b) and into the union of the planes $k_y = \pi$ and $k_z = 0$ shown in (c).

$\nu(P')$, $\nu(P'')$ defined. The projection operator, P can be decomposed as in Eq. (1.1) and written as $P = P_1 + P_2$ where $P_1 = P_1' \oplus P_1''$ and $P' = P_1' \oplus P_2'$ etc. where we again assume that the decomposition is such that P_1, P_1', P_1'' etc. are globally smooth on their domains of definition so that the corresponding Chern numbers are well defined.

It follows that

$$\nu(P) = \nu(P') + \nu(P'') = \nu_2 + \tilde{\nu_3}. \tag{2.1}$$

Consider now, a continuous deformation of the surface parameterized by a variable, t, which varies from 0 to 1 such that at every point of the deformation, the surface $S(t)$ gets mapped onto itself under inversion. $S(0)$ corresponds to the surface previously denoted by S. A possible value of $S(t)$ for $0 < t < 1$ is shown in Fig. 1(b). At $t = 1$, the surface $S(t)$

becomes the surface shown in Fig. 1(c). This surface is the union of the planes $k_y = \pi$ and $k_z = 0$. Under this transformation, the projection operator which becomes a continuous function of t, $P(t)$ also changes continuously and the Z_2 invariant therefore does not change. (Note however, that we do not require that $P_1(t,k)$ is a smooth function of t.)

Thus, it follows that

$$\nu(P(1)) = \nu(P(0)) = \nu(P). \tag{2.2}$$

Further, since $S(1)$ can be regarded as the union of the planes $k_y = \pi$ and $k_z = 0$,

$$\nu(P(1)) = \tilde{\nu}_2 + \nu_3. \tag{2.3}$$

Thus, from Eqs. (2.1),(2.2) and (2.3), we conclude that

$$\nu_2 - \tilde{\nu}_2 = \nu_3 - \tilde{\nu}_3.$$

The plane $k_z = k_y$ can also be obtained as a deformation of the surface in Fig. 1(b). Thus the Z_2 invariant of this plane is obtained as $\tilde{\nu}_2 + \nu_3$. Similarly, by deforming surfaces S' which we define as the union of the planes $k_x = 0$ and $k_y = \pi$ and S'' which we define as the union of the planes $k_x = 0$ and $k_z = \pi$ it can easily be shown that

$$\nu_1 - \tilde{\nu}_1 = \nu_2 - \tilde{\nu}_2 = \nu_3 - \tilde{\nu}_3. \tag{2.4}$$

Further, the Z_2 invariant of any other plane which maps onto itself under TRS can also be obtained from the values of ν_1, ν_2, ν_3 and $\nu_1 - \tilde{\nu}_1$. We can thus characterize any topological insulator with TRS in three dimensions with four invariants, which may be chosen to be ν_1, ν_2, ν_3 and $|\nu_1 - \tilde{\nu}_1|$.

The arguments in Ref. 9 may be summarized as follows. The spectral projection operator in 3d when restricted to the planes $k_i = 0, k_i = \pi$ for $k_i \in \{k_x, k_y, k_z\}$ can be written as a sum $P = P_1 + P_2$, where P_1, P_2 map onto each other under TRS.

Consider the set of momentum space slices, $k_z = c$, where $0 \le c \le \pi$. Let $P_1(c), P_2(c)$ be the restriction of the operators P_1 and P_2 to the plane $k_z = c$. For an arbitrary value of c, these operators do not map onto each other under TRS. The Z_2 invariant is therefore not well defined in general. When the Z_2 invariants for the planes $k_z = 0$, $k_z = \pi$ are different, the operators, $P_1(0)$ and $P_1(\pi)$ have different Chern numbers. A continuous deformation of a two dimensional projection operator to one which has a different Chern number is not possible. Changes in Chern number may be regarded as occurring at singular diabolical

points or monopoles at which the projection operator is not well defined. In general, one may define 2d surfaces enclosing points at which the projection operators P_1, P_2 are not well defined and associate a charge with these surfaces. If the difference in Chern number of P_1 on the slice $k_z = 0$ to the Chern number of P_1 on the slice $k_z = \pi$ is an odd integer, this implies the existence of a net odd monopole charge between these two planes and ensures that the Z_2 invariants of the planes $k_z = 0$ and $k_z = \pi$ are different. By a careful counting of monopole charges and by using TRS, one can then show that in this case, the Z_2 invariants of the $k_x = 0$ and $k_x = \pi$ planes also differ from each other and the same is true for the $k_y = 0$ and $k_y = \pi$ planes.

This fourth Z_2 invariant, $\nu_1 - \tilde{\nu}_1$ is an intrinsically three dimensional characteristic of the insulator. Insulators whose fourth Z_2 invariant is zero and one have been christened "weak" and "strong" topological insulators respectively. The four invariants found here agree with the counting in Refs. 8,11.

In summary, we have analyzed the Chern number formula for the Z_2 invariant in two dimensions. The trivial and non-trivial topological classes may be thought of as equivalence classes of Hamiltonians which contain respectively members with even and an odd quantized spin Hall conductance. A simple counting argument for the number of invariants in 3d was provided using deformations of planes which map onto themselves under time reversal.

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